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High P-T experiments and first principles calculations of Si, O, Cr diffusion in liquid iron

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Chemical diffusion of alloying elements in liquid iron is important for understanding the kinetics of metal-silicate equilibration during core formation, compositional buoyancy of liquid iron alloys from inner-core crystallization, and chemical interaction at planetary core-mantle boundaries during cooling. We have measured the pressure and temperature dependences of Si, O, and Cr chemical diffusion in molten iron both experimentally at 1–18 GPa and 1873–2423 K using a multianvil apparatus, and theoretically from ambient pressure to 135 GPa and 2200–5000 K using first principles molecular dynamic calculations. Our findings corroborate theoretical estimates that diffusion coefficients are scalable to the absolute melting temperature (T_m) yielding constant diffusivities of approximately $4.0 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$ along the melting curve from ambient to Earth-core pressures. Arrhenian activation terms for Si, O, and Cr chemical diffusion are consistent with theoretical data but appreciably smaller than previously reported experimental values for Fe and alloying element self-diffusion in liquid iron and iron alloys derived from much smaller data sets.

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